Exploring the Structural Basis of Substrate Preferences in Baeyer-Villiger Monooxygenases INSIGHT FROM STEROID MONOOXYGENASE

Franceschini, Stefano; van Beek, Hugo L.; Pennetta, Alessandra; Martinoli, Christian; Fraaije, Marco W.; Mattevi, Andrea

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SUPPLEMENTAL DATA

Exploring the structural basis of substrate preferences in Baeyer-Villiger monooxygenases: insight from steroid monooxygenase

Stefano Franceschini[1], Hugo L. van Beek[2], Alessandra Pennetta[1], Christian Martinoli[1],

Marco W. Fraaije[2]*, Andrea Mattevi[1]*

[1] Department of Biology and Biotechnology, University of Pavia, Via Ferrata 9, 27100 Pavia, Italy

[2] Laboratory of Biochemistry, Groningen Biomolecular Sciences and Biotechnology Institute, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Running Title: Steroid monooxygenase from *Rhodococcus rhodochrous*

SUPPLEMENTARY FIGURES

Figure S1. Quality of the final electron density with reference to the crystal structure of STMO bound to $NADP^+$ (Table 1). The density was calculated with weighted 2Fo-Fc coefficients and is contoured at 1.3 σ level. Carbons are in purple, nitrogens in blue, oxygens in red, sulfurs in yellow, and phosphorous in orange.

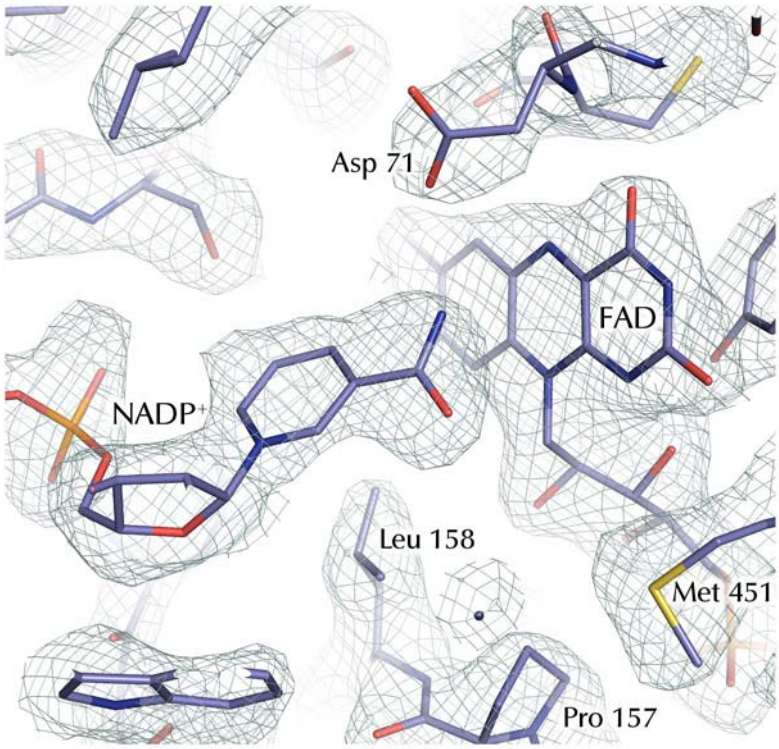

Figure S2. Superposition of STMO (blue ribbon) and CHMO (green ribbon; open conformation; PDB entry 3GWF) active sites. FAD and $NADP^+$ of STMO are depicted with yellow and orange carbons, respectively. The Cα atoms of the STMO residues targeted by mutagenesis are shown as blue spheres (Table 3).